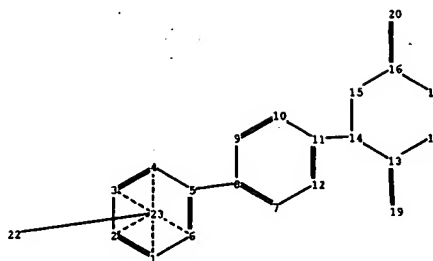
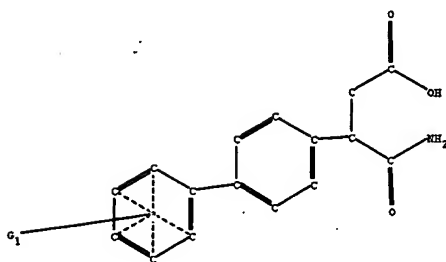


hll
3/22/2007



chain nodes :

13 14 15 16 17 18 19 20 22 24 25 27 28 30 31 32 33 34

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

5-8 11-14 13-14 13-18 13-19 14-15 15-16 16-17 16-20 24-25 27-31 28-32 30-34 33-34

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

13-18 13-19 27-31 28-32 30-34 33-34

exact bonds :

5-8 11-14 13-14 14-15 15-16 24-25

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 16-17 16-20

G1:H,X,CN,NO2,[*1],[*2],[*3],[*4]

G2:H,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:CLASS14:CLASS15:CLASS16:CLASS17:CLASS18:CLASS19:CLASS20:CLASS22:CLASS23:Atom
24:CLASS

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hu
3/22/07

=>

Uploading C:\Program Files\Stnexp\Queries\2007 cases\10569812\Formula(Ia) c15.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam

SAMPLE SEARCH INITIATED 19:00:08 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 17 TO ITERATE

100.0% PROCESSED 17 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 93 TO 587

PROJECTED ANSWERS: 0 TO 0

L2

0 SEA SSS SAM L1

=> s l1 sss ful

FULL SEARCH INITIATED 19:00:13 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 354 TO ITERATE

100.0% PROCESSED 354 ITERATIONS

6 ANSWERS

SEARCH TIME: 00.00.01

L3

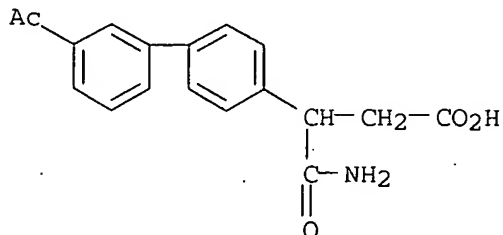
6 SEA SSS FUL L1

=> d scan

L3 6 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN [1,1'-Biphenyl]-4-propanoic acid, 3'-acetyl-β-(aminocarbonyl)- (9CI)

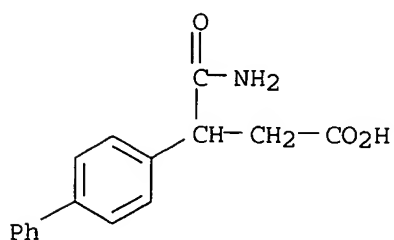
MF C18 H17 N O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

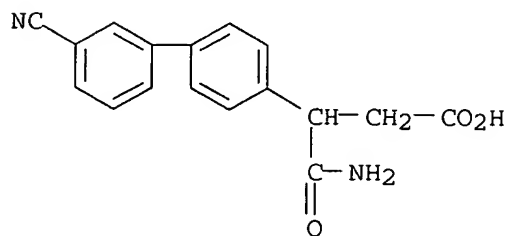
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):6

L3 6 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN [1,1'-Biphenyl]-4-propanoic acid, β -(aminocarbonyl)- (9CI)
MF C16 H15 N O3



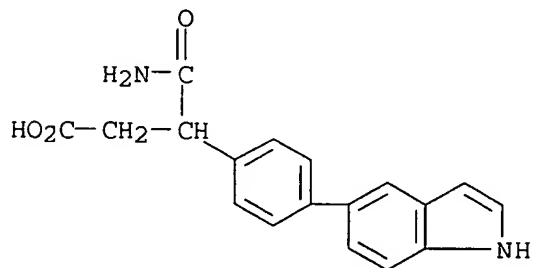
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 6 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN [1,1'-Biphenyl]-4-propanoic acid, β -(aminocarbonyl)-3'-cyano- (9CI)
MF C17 H14 N2 O3



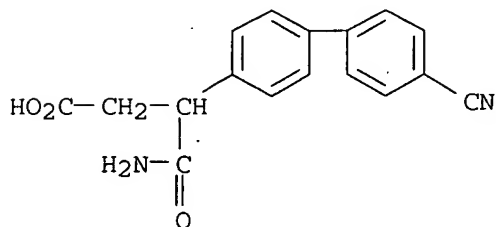
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 6 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benzenepropanoic acid, β -(aminocarbonyl)-4-(1H-indol-5-yl)- (9CI)
MF C18 H16 N2 O3



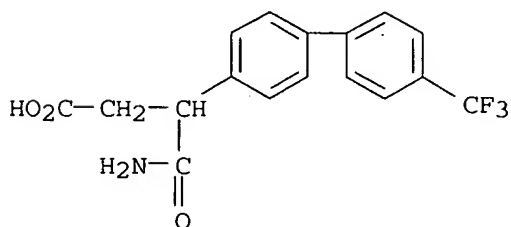
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 6 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN [1,1'-Biphenyl]-4-propanoic acid, β -(aminocarbonyl)-4'-cyano- (9CI)
MF C17 H14 N2 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 6 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN [1,1'-Biphenyl]-4-propanoic acid, β -(aminocarbonyl)-4'-(trifluoromethyl)- (9CI)
MF C17 H14 F3 N O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=>

=> fil hcap
COST IN U.S. DOLLARS
FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
172.55	172.76

FILE 'HCAPLUS' ENTERED AT 19:00:52 ON 22 MAR 2007
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FILE COVERS 1907 - 22 Mar 2007 VOL 146 ISS 13

FILE LAST UPDATED: 21 Mar 2007 (20070321/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 18:59:11 ON 22 MAR 2007)

FILE 'REGISTRY' ENTERED AT 18:59:32 ON 22 MAR 2007

L1 STRUCTURE UPLOADED
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L3 6 S L1 SSS FUL

FILE 'HCAPLUS' ENTERED AT 19:00:52 ON 22 MAR 2007

=> s l3

L4 1 L3

=> d l4 ibib abs

L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:158625 HCAPLUS
DOCUMENT NUMBER: 142:261292
TITLE: Preparation of (hetero)aryl-substituted succinate derivatives as matrix metalloproteinase inhibitors
INVENTOR(S): Holmes, Ian; Watson, Stephen Paul
PATENT ASSIGNEE(S): Glaxo Group Limited, UK
SOURCE: PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005016868	A2	20050224	WO 2004-EP9087	20040812
WO 2005016868	A3	20050519		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,				

10/569812MMP Inhibitors Formula Ia c15

LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1654218 A2 20060510 EP 2004-764084 20040812
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JP 2007502259 T 20070208 JP 2006-522996 20040812

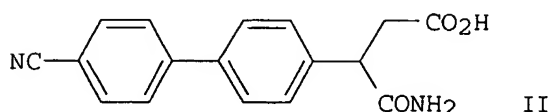
US 2006235074 A1 20061019 US 2006-569812 20060210

PRIORITY APPLN. INFO.: GB 2003-19069 A 20030814

WO 2004-EP9087 W 20040812

OTHER SOURCE(S): CASREACT 142:261292; MARPAT 142:261292

GI



AB Title compds. represented by the formula I, R1ZQCH(R2)CH2X, [wherein R1 = (un)substituted alkyl(cycloalkyl), alkylheterocycloalkyl, alkylaryl, etc.; Z = a bond, CH2, O, S, etc.; Q = (un)substituted (hetero)aryl; X = COR3; R2 = CONH2, CO2H, sulfonylamino, etc.; R3 = OH, oxyalkyl or (un)substituted amino; with a proviso; and physiol. functional derivs. thereof] were prepared as matrix metalloproteinase (MMP) inhibitors. Coupling reaction of 4-amino-3-(4-bromophenyl)-4-oxobutanoic acid with p-nitrilephenylboronic acid gave II in 100% yield. I showed inhibition of MMP-12 with IC50 values of below 100 µM. Thus, I and their pharmaceutical compns. are useful as matrix metalloproteinase inhibitors for the treatment of inflammation or autoimmune disease (no data).

10/569812MMP Inhibitors PGPUb search

hwe
3/21/07

845786-10-9P 845786-11-0P 845786-12-1P 845786-13-2P 845786-14-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of (hetero)aryl-substituted succinate derivs. as matrix
metalloproteinase inhibitors)

ALL ANSWERS HAVE BEEN SCANNED

=> d his

(FILE 'HOME' ENTERED AT 18:59:11 ON 22 MAR 2007)

FILE 'REGISTRY' ENTERED AT 18:59:32 ON 22 MAR 2007

L1 STRUCTURE UPLOADED
L2 0 S L1 SSS SAM
L3 6 S L1 SSS FUL

FILE 'HCAPLUS' ENTERED AT 19:00:52 ON 22 MAR 2007

L4 1 S L3

FILE 'HCAPLUS' ENTERED AT 19:04:22 ON 22 MAR 2007

E US20060235074/PN,PRN,AN
L5 1 S E3

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
5.20	196.39

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-0.78

CA SUBSCRIBER PRICE

3/23/07

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 E5 0 US2006235074/AN
 E6 1 US2006235075/PN
 E7 1 US2006235076/PN
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 E9 2 US2006235078/PN
 E10 1 US2006235079/PN
 E11 1 US2006235080/PN
 E12 1 US2006235081/PN

=> s e3

L5 1 US2006235074/PN

=> d scan

L5 1 ANSWERS HCAPLUS COPYRIGHT 2007 ACS on STN

IC ICM C07C235-00

CC 25-2 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 Section cross-reference(s): 1, 63

TI Preparation of (hetero)aryl-substituted succinate derivatives as matrix metalloproteinase inhibitors

ST hetero aryl butanoic acid prepn MMP inhibitor antiinflammation immunomodulator

IT Anti-inflammatory agents

Autoimmune disease

Drug delivery systems

Human

Immunomodulators

Inflammation

(preparation of (hetero)aryl-substituted succinate derivs. as matrix metalloproteinase inhibitors)

IT 845786-15-4P 845786-16-5P 845786-17-6P 845786-18-7P 845786-19-8P
 845786-20-1P 845786-21-2P 845786-22-3P 845786-23-4P 845786-24-5P
 845786-25-6P 845786-26-7P 845786-27-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of (hetero)aryl-substituted succinate derivs. as matrix metalloproteinase inhibitors)

IT 107-82-4, 1-Bromo-3-methylbutane 156-38-7, p-Hydroxyphenylacetic acid
 1647-26-3, 2-Cyclohexylethyl bromide 1878-68-8, 4-Bromophenylacetic acid
 5292-43-3, tert-Butyl bromoacetate 5437-45-6, Benzyl 2-bromoacetate
 14199-15-6, Methyl 2-(4-hydroxyphenyl)acetate 18162-48-6,
 tert-Butyldimethylsilyl chloride 27727-37-3, Benzyl 2-(4-hydroxyphenyl)acetate 98946-18-0 126747-14-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of (hetero)aryl-substituted succinate derivs. as matrix metalloproteinase inhibitors)

IT 33155-58-7P, tert-Butyl 2-(4-bromophenyl)acetate 55784-09-3P,
 [4-(Isopentyloxy)phenyl]acetic acid 127152-98-1P, Benzyl

2-(4-bromophenyl)acetate 335200-36-7P 845785-97-9P 845785-98-0P
 845785-99-1P 845786-00-7P 845786-01-8P 845786-02-9P 845786-03-0P
 845786-04-1P 845786-06-3P 845786-07-4P 845786-08-5P 845786-09-6P

Reg Nos.

10/569812MMP Inhibitors REG NO. search

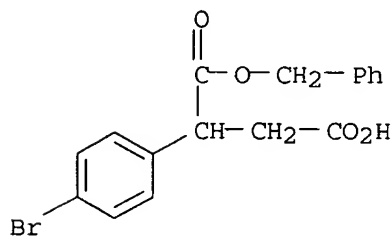
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845786-04-1/rn

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RN OR 845786-03-0/RN OR 845786-04-1/RN

=> d scan

L1 9 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Butanedioic acid, (4-bromophenyl)-, 1-(phenylmethyl) ester (9CI)
MF C17 H15 Br O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):9

L1 9 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Butanedioic acid, (4-bromophenyl)-, 1-(1,1-dimethylethyl) 4-(phenylmethyl)
ester (9CI)
MF C21 H23 Br O4

